Volume 13 | Number 20 | 28 May 2015 | Pages 5559–5832

Organic & Biomolecular Chemistry

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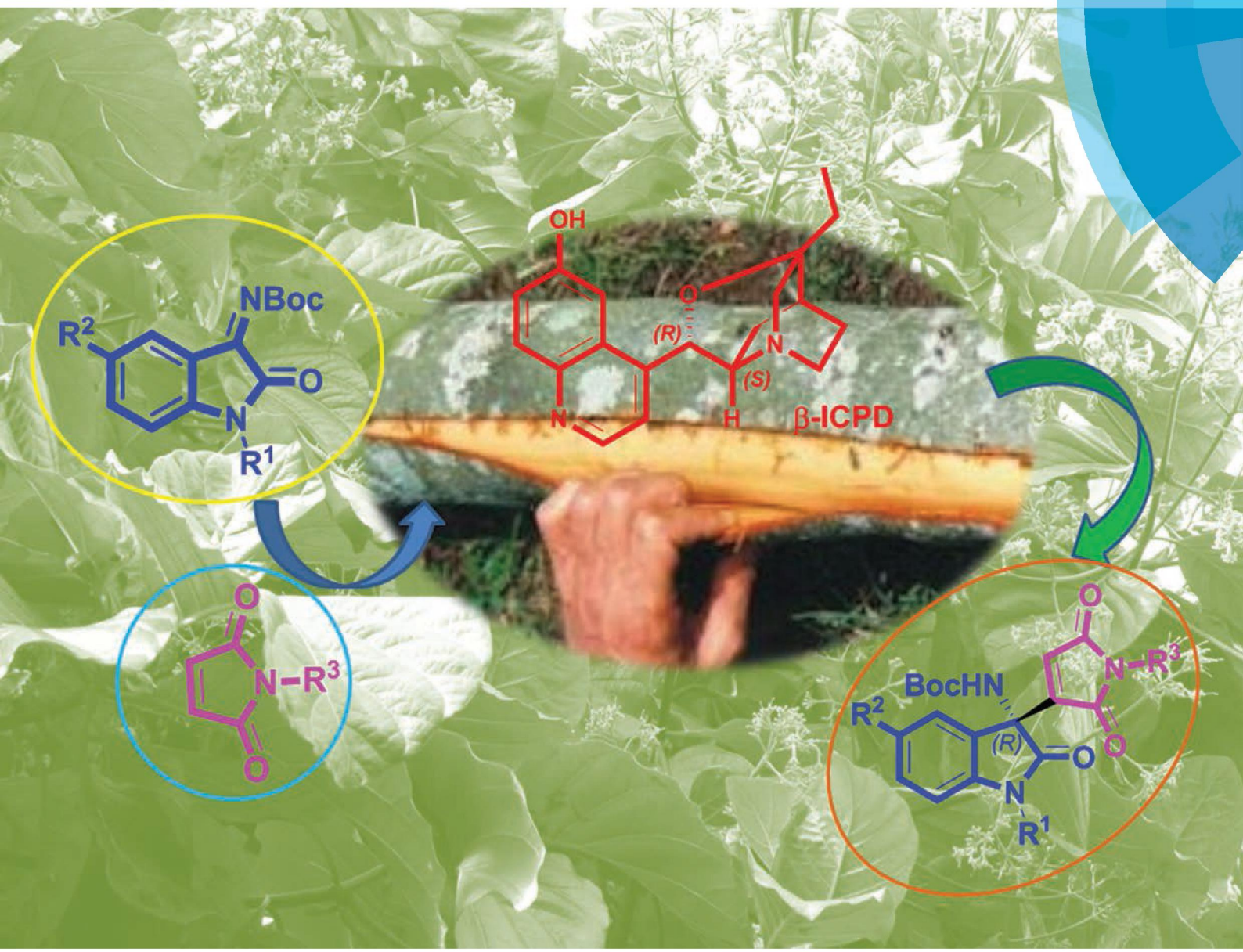

ISSN 1477-0520

ROYAL SOCIETY OF CHEMISTRY

PAPER

Swapandeep Singh Chimni *et al.*

Maleimide as an efficient nucleophilic partner in the aza-Morita–Baylis–Hillman reaction: synthesis of chiral 3-substituted-3-aminooxindoles

Organic & Biomolecular Chemistry

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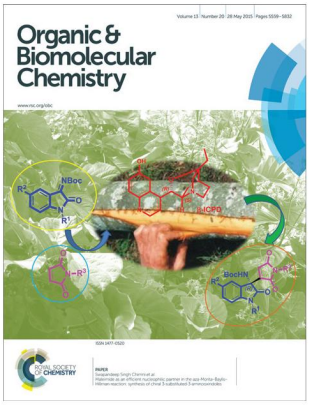
IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 13(20) 5559–5832 (2015)



Cover
See Swapandeep Singh Chimni *et al.*, pp. 5629–5635.

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Inside cover
See Joshua S. Mylne, Keith A. Stubbs *et al.*, pp. 5586–5590.

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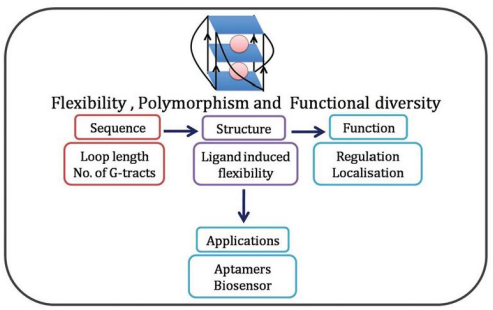
REVIEW

5570

The tale of RNA G-quadruplex

Prachi Agarwala, Satyaprakash Pandey and Souvik Maiti*

The RNA secondary structure G-quadruplex with its malleable nature can execute diverse biological functions and can be manipulated and used for various applications.



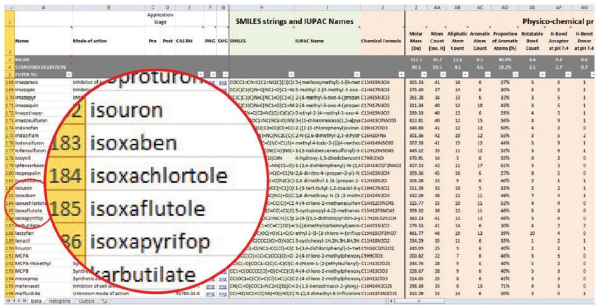
COMMUNICATIONS

5586

An interactive database to explore herbicide physicochemical properties

Michael N. Gandy, Maxime G. Corral, Joshua S. Mylne* and Keith A. Stubbs*

An interactive database containing the physicochemical properties of successful herbicidal compounds that allows rapid comparison to potential, new herbicidal compounds is presented.



Organic & Biomolecular Chemistry (print: ISSN 1477-0520; electronic: ISSN 1477-0539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

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Organic & Biomolecular Chemistry

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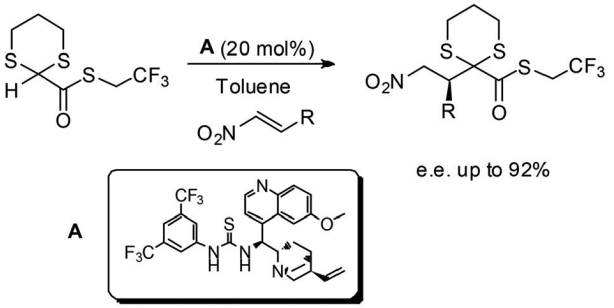
COMMUNICATIONS

5591

Stereoselective reaction of 2-carboxythioesters-1,3-dithiane with nitroalkenes: an organocatalytic strategy for the asymmetric addition of a glyoxylate anion equivalent

E. Massolo, M. Benaglia,* A. Genoni, R. Annunziata, G. Celentano and N. Gaggero*

Under mild reaction conditions γ-nitro-β-aryl-α-keto esters with up to 92% ee were obtained, realizing a formal catalytic stereoselective conjugate addition of the glyoxylate anion synthon.

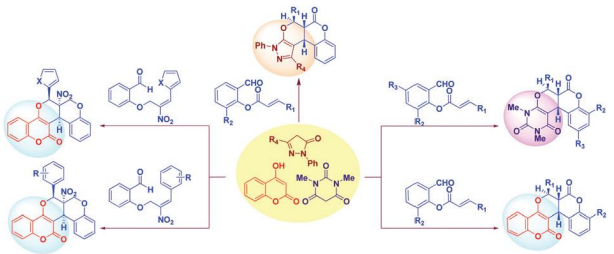


5597

Stereoselective construction of functionalized tetracyclic and pentacyclic coumarinopyranpyrazole/pyrimidinedione/coumarin scaffolds using a solid-state melt reaction

Manickam Bakthadoss,* Damodharan Kannan, Nagappan Sivakumar, Palani Malathi and Vasudevan Manikandan

An assembly of tetra / pentacyclic hybrid scaffolds have been synthesized for the first time using a solid-state melt reaction in a stereoselective fashion with excellent yields.

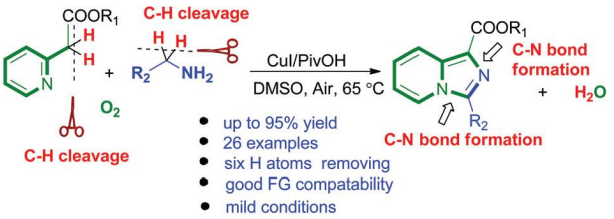


5602

Copper-catalyzed aerobic oxidative amination of C(sp^3)–H bonds: synthesis of imidazo[1,5-*a*]-pyridines

Darapaneni Chandra Mohan, Sadu Nageswara Rao, Chitrakar Ravi and Subbarayappa Adimurthy*

Copper-catalyzed synthesis of imidazo[1,5-*a*]pyridine-1-carboxylates through oxidative amination of C(sp^3)–H bonds under mild aerobic conditions with broad substrate scope has been achieved.

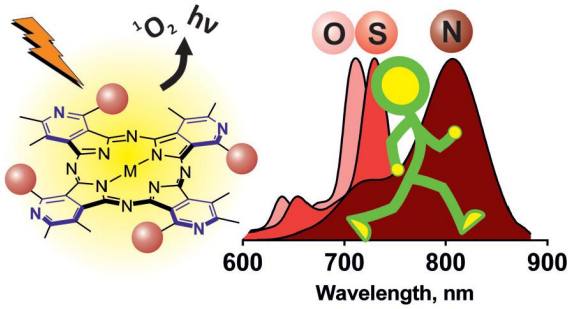


5608

Heteroatom-substituted tetra(3,4-pyrido)-porphyrazines: a stride toward near-infrared-absorbing macrocycles

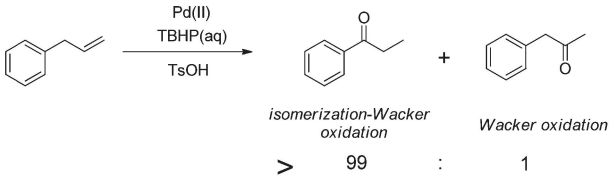
Lenka Vachova, Miloslav Machacek, Radim Kučera, Jiri Demuth, Pavel Cermak, Kamil Kopecky, Miroslav Miletin, Adela Jedlickova, Tomas Simunek, Veronika Novakova* and Petr Zimcik*

Synthesis and photophysical properties are reported for substituted tetra(3,4-pyrido)porphyrazines that absorb light as far as at 800 nm.



COMMUNICATIONS

5613

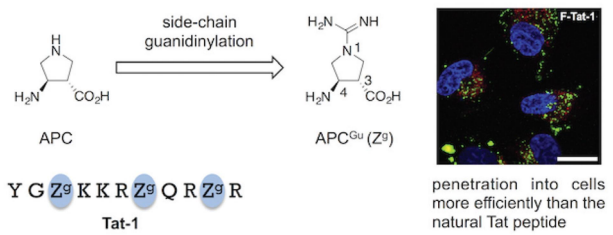


Direct conversion of allyl arenes to aryl ethylketones *via* a TBHP-mediated palladium-catalyzed tandem isomerization–Wacker oxidation of terminal alkenes

JinWu Zhao, Li Liu,* ShiJian Xiang, Qiang Liu and HuoJi Chen*

A TBHP-mediated palladium-catalyzed tandem isomerization–Wacker oxidation of terminal alkenes was developed.

5617

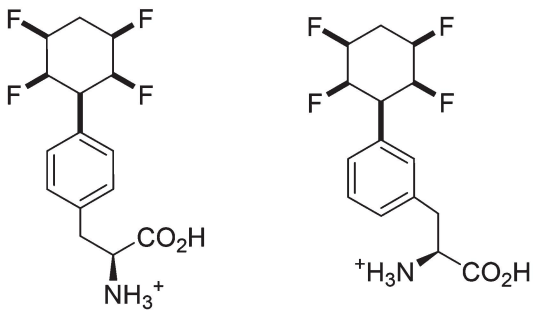


A preorganized β-amino acid bearing a guanidinium side chain and its use in cell-penetrating peptides

Yosuke Demizu,* Makoto Oba, Koyo Okitsu, Hiroko Yamashita, Takashi Misawa, Masakazu Tanaka, Masaaki Kurihara and Samuel H. Gellman

A cyclic β-amino acid (APC^{Gu}) bearing a side-chain guanidinium group has been developed.

5621

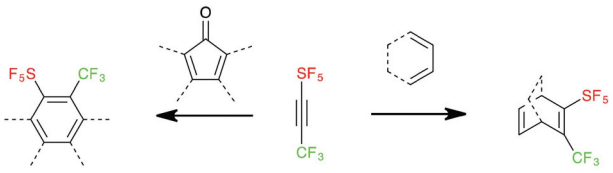


Fluorine containing amino acids: synthesis and peptide coupling of amino acids containing the all-*cis* tetrafluorocyclohexyl motif

Mohammed Salah Ayoup, David B. Cordes, Alexandra M. Z. Slawin and David O'Hagan*

A synthesis of amino acids carrying the all-*cis* tetrafluorocyclohexyl ring moiety is demonstrated and protection/deprotection elaborations are illustrated which show that this facially polarised ring motif may be incorporated into peptides.

5625



Simultaneous introduction of trifluoromethyl and λ⁶-pentafluorosulfanyl substituents using $F_5S{-}C{\equiv}C{-}CF_3$ as a dienophile

Blazej Duda* and Dieter Lentz*

$SF_5{-}C{\equiv}C{-}CF_3$ as a powerful dienophile in Diels–Alder reactions, provides the corresponding products in up to quantitative yields and allows the introduction of the pentafluorosulfanyl group and trifluoromethyl group at the 1,2 position.

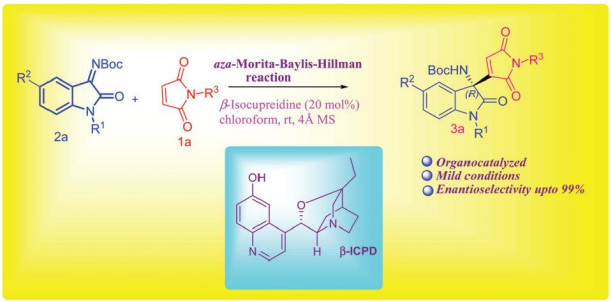
PAPERS

5629

Maleimide as an efficient nucleophilic partner in the aza-Morita–Baylis–Hillman reaction: synthesis of chiral 3-substituted-3-aminooxindoles

Akshay Kumar, Vivek Sharma, Jasneet Kaur, Naveen Kumar and Swapandeep Singh Chimni*

A highly enantioselective β-isocupreidine catalyzed aza-Morita–Baylis–Hillman reaction of maleimides with isatin derived ketimines provides 3-substituted-3-aminooxindoles with enantiomeric excess upto 99%.

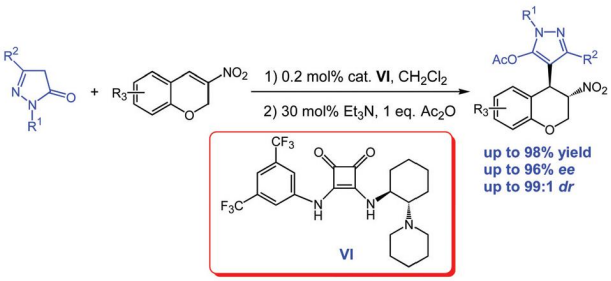


5636

Enantioselective synthesis of chiral heterocycles containing both chroman and pyrazolone derivatives catalysed by a chiral squaramide

Jun-Hua Li and Da-Ming Du*

An efficient chiral squaramide-catalysed enantioselective Michael addition of pyrazolin-5-ones to 3-nitro-2*H*-chromenes afforded chiral heterocycles containing both chroman and pyrazolone derivatives in high to excellent yields (up to 98%) with high enantioselectivities (up to 96%) under very low catalyst loading (0.2 mol%).

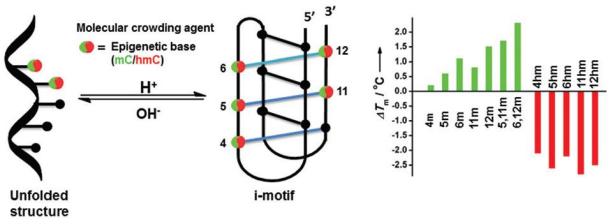


5646

Regulation of telomeric i-motif stability by 5-methylcytosine and 5-hydroxymethylcytosine modification

Baochang Xu, Gitali Devi and Fangwei Shao*

Thermal denaturation of a C-rich DNA sequence substituted with mC or hmC under various acidic pH indicate that DNA i-motif is stabilized by one or two mCs, but is destabilized by either single modification with hmC or hypermethylation with mC.

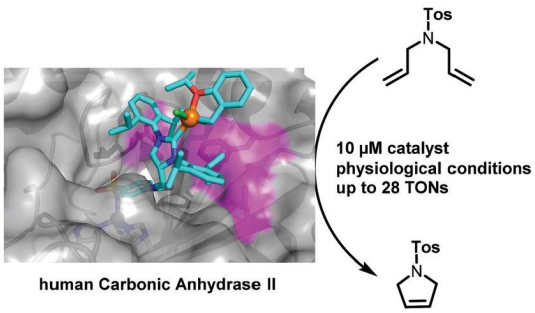


5652

Carbonic anhydrase II as host protein for the creation of a biocompatible artificial metathesase

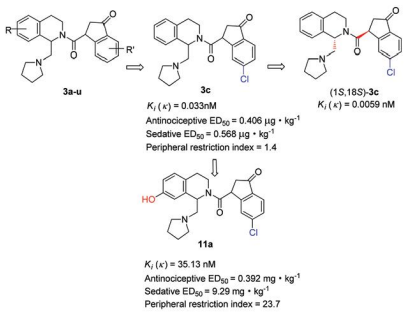
Jingming Zhao, Anna Kajetanowicz and Thomas R. Ward*

We report an efficient artificial metathesase which combines an arylsulfonamide anchor within the protein scaffold human carbonic anhydrase II.



PAPERS

5656

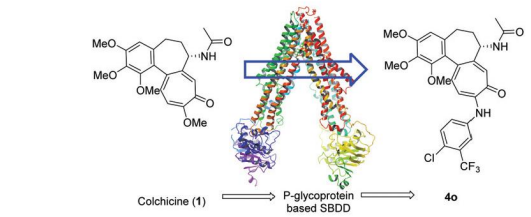


Discovery, stereospecific characterization and peripheral modification of 1-(pyrrolidin-1-ylmethyl)-2-[(6-chloro-3-oxo-indan)-formyl]-1,2,3,4-tetrahydroisoquinolines as novel selective κ opioid receptor agonists

Z.-J. Gan, Y.-H. Wang, Y.-G. Xu,* T. Guo, J. Wang, Q. Song, X.-J. Xu, S.-Y. Hu, Y.-J. Wang, D.-C. Wang, D.-Z. Sun, D. Zhang, T. Xi, H.-D. Li, H.-B. Zhang, T.-J. Hang, H.-G. Lu and J.-G. Liu*

11a produces potent peripheral antinociception.

5674



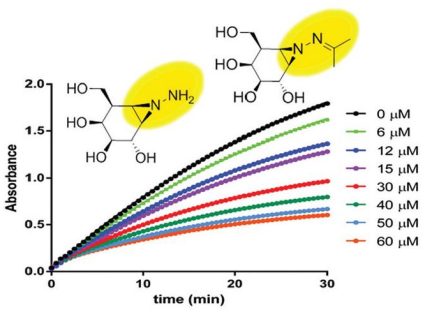
HCT-116, IC_{50} (nM)	50	40
Pgp induction, EC_{50} (nM)	14.4	69
% TGI at 1.25 mg/kg, p.o. (Ehrlich solid tumor model)	29.91	34.10

Colchicine derivatives with potent anticancer activity and reduced P-glycoprotein induction liability

B. Singh, A. Kumar, P. Joshi, S. K. Guru, S. Kumar, Z. A. Wani, G. Mahajan, A. Hussain, A. K. Qazi, A. Kumar, S. S. Bharate, B. D. Gupta, P. R. Sharma, A. Hamid, A. K. Saxena, D. M. Mondhe, S. Bhushan, S. B. Bharate* and R. A. Vishwakarma*

Colchicine derivatives with reduced P-gp induction liability have been identified.

5690

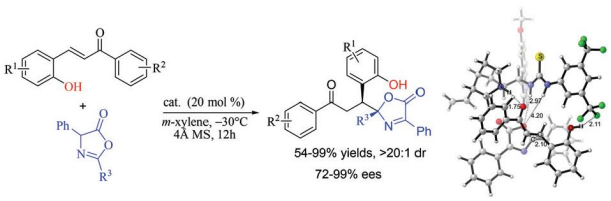


Galacto configured *N*-aminoaziridines: a new type of irreversible inhibitor of β-galactosidases

Anna Alcaide, Ana Trapero, Yolanda Pérez and Amadeu Llebaria*

N-Aminoaziridines are potent irreversible inhibitors of galactosidases.

5698



Organocatalytic regioselective asymmetric Michael addition of azlactones to *o*-hydroxy chalcone derivatives

Shao-Yun Zhang, Gui-Yu Ruan, Zhi-Cong Geng, Nai-Kai Li, Ming Lv, Yong Wang* and Xing-Wang Wang*

Regio- and enantio-selective Michael addition between azlactones with *o*-hydroxy chalcone derivatives is reported. Optically active *N*,*O*-aminals are obtained in good yields with good to excellent diastereo- and enantio-selectivities.

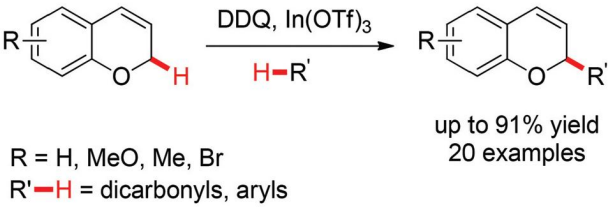
PAPERS

5710

Indium-catalyzed oxidative cross-dehydrogenative coupling of chromenes with 1,3-dicarbonyls and aryl rings

Fanmei Li, Zhilin Meng, Jing Hua, Wei Li, Hongxiang Lou and Lei Liu*

An efficient indium-catalyzed oxidative cross-dehydrogenative coupling of chromenes with 1,3-dicarbonyls and aryl rings promoted by DDQ was described.

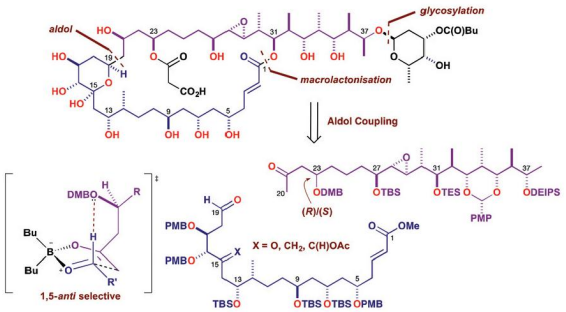


5716

Synthetic studies toward the brasilinolides: controlled assembly of a protected C1–C38 polyol based on fragment union by complex aldol reactions

Ian Paterson,* Michael P. Housden, Christopher J. Cordier, Paul M. Burton, Friedrich A. Mühlthau and Olivier Loiseleur

A modular strategy for the synthesis of the immunosuppressant macrolide brasilinolide A was adopted based on coupling suitable northern and southern fragments.

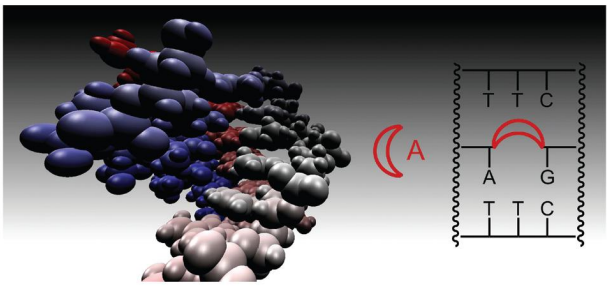


5734

Effect of preorganization on the affinity of synthetic DNA binding motifs for nucleotide ligands

S. Vollmer and C. Richert*

Triple helices with an abasic bridge between two oligopurine segments bind ligands like ATP, FAD, and cAMP with dissociation constants as low as 30 nM.

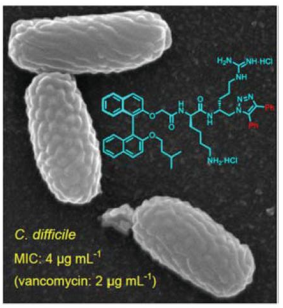


5743

Binaphthyl-1,2,3-triazole peptidomimetics with activity against *Clostridium difficile* and other pathogenic bacteria

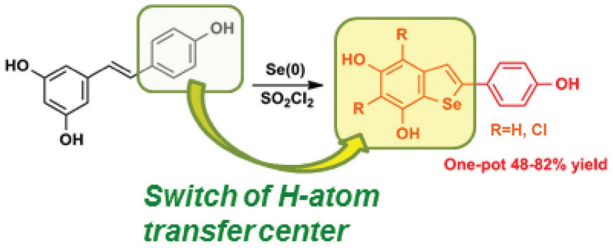
Steven M. Wales, Katherine A. Hammer, Amy M. King, Andrew J. Tague, Dena Lyras, Thomas V. Riley, Paul A. Keller* and Stephen G. Pyne*

Designed binaphthyl-based, cationic peptidomimetic antimicrobials targeting *C. difficile*, incorporating a click-derived 1,2,3-triazole ester isostere at the C-terminus MICs of 4 μg mL^{-1} against three human isolates of *C. difficile*.



PAPERS

5757

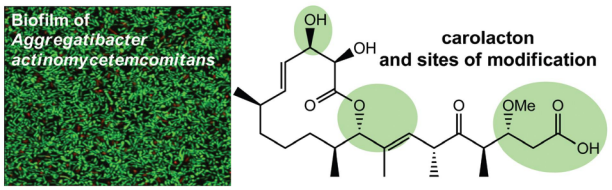


Resveratrol-based benzoselenophenes with an enhanced antioxidant and chain breaking capacity

Damiano Tanini, Lucia Panzella,* Riccardo Amorati, Antonella Capperucci,* Elio Pizzo, Alessandra Napolitano, Stefano Menichetti and Marco d'Ischia

One-pot selenenylation of resveratrol with Se(0) and SO_2Cl_2 leads to benzoselenophene derivatives with efficient Trolox-like antioxidant and chain breaking capacity.

5765

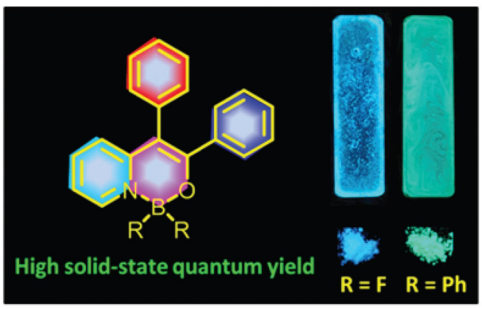


Synthesis of new carolacton derivatives and their activity against biofilms of oral bacteria

N. Stumpp, P. Premnath, T. Schmidt, J. Ammermann, G. Dräger, M. Reck, R. Jansen, M. Stiesch,* I. Wagner-Döbler* and A. Kirschning*

Carolacton, a secondary metabolite isolated from the extracts of *Sorangium cellulosum*, causes membrane damage and cell death in biofilms of different oral bacteria.

5775

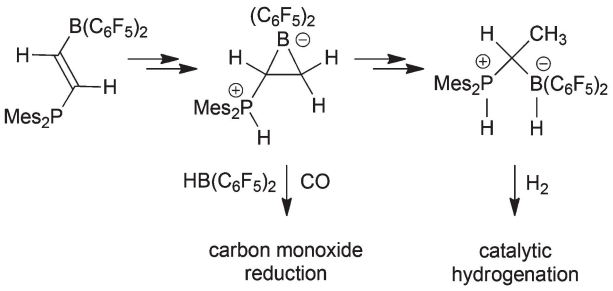


High solid-state luminescence in propeller-shaped AIE-active pyridine–ketoiminate–boron complexes

Yanping Wu, Zhenyu Li, Qingsong Liu, Xiaoqing Wang,* Hui Yan, Shuwen Gong, Zhipeng Liu* and Weijiang He*

Two pyridine-ketoiminate-based organoboron complexes were demonstrated to possess aggregation-induced emission, large Stokes shift and high quantum yield in the solid-state, which were rationalized through X-ray crystal analysis and electronic structure calculations.

5783



Direct synthesis of a geminal zwitterionic phosphonium/hydridoborate system – developing an alternative tool for generating frustrated Lewis pair hydrogen activation systems

Jiangang Yu, Gerald Kehr, Constantin G. Daniliuc, Christoph Bannwarth, Stefan Grimme and Gerhard Erker*

A convenient way to a new class of geminal $Mes_2PH^+/B(C_6F_5)_2H^-$ pairs is presented.

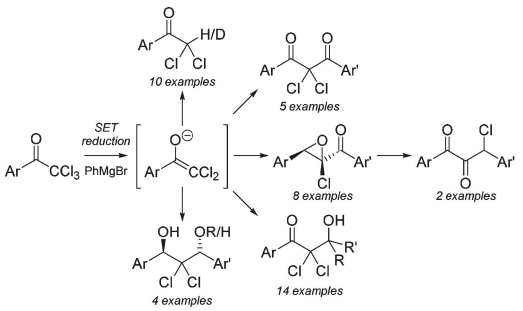
PAPERS

5793

Grignard-mediated reduction of 2,2,2-trichloro-1-arylethanones

Ali H. Essa, Reinner I. Lerrick, Eçe Çiftçi, Ross W. Harrington, Paul G. Waddell, William Clegg and Michael J. Hall*

2,2,2-Trichloro-1-aryl-ethanones can be reduced by RMgX to the corresponding 2,2-dichloro-1-arylethen-1-olates and trapped with a range of electrophiles. In addition we demonstrate that 2,2-dichloro-1-arylethen-1-olates undergo counter-ion controlled Darzens condensations.

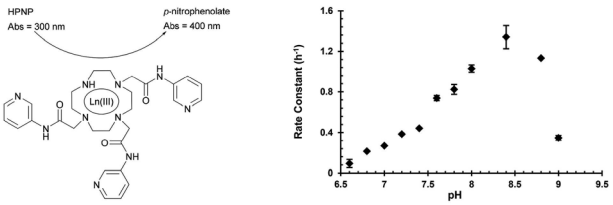


5804

Tri- and tetra-substituted cyclen based lanthanide(III) ion complexes as ribonuclease mimics: a study into the effect of log K_a, hydration and hydrophobicity on phosphodiester hydrolysis of the RNA-model 2-hydroxypropyl-4-nitrophenyl phosphate (HPNP)

Ann-Marie Fanning, Sally. E. Plush* and Thorfinnur Gunnlaugsson*

Lanthanide(III) complexes of 'pseudo' dipeptide ligands and 3'-pyridine ligands have been characterised as metallo-ribonuclease mimics.

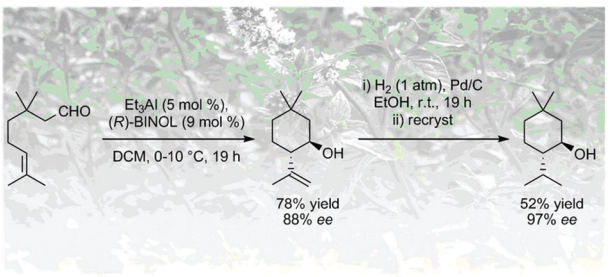


5817

BINOL-Al catalysed asymmetric cyclization and amplification: preparation of optically active menthol analogs

Hisanori Itoh, Hironori Maeda, Shinya Yamada, Yoji Hori,* Takashi Mino* and Masami Sakamoto

We report a highly selective asymmetric ring-closing ene reaction catalyzed by chiral aluminum complexes. Asymmetric amplification of this reaction was investigated by varying the ee of the BINOL employed in the catalyst.



5826

Palladium-catalyzed asymmetric allylic amination of racemic butadiene monoxide with isatin derivatives

Gen Li, Xiangqing Feng* and Haifeng Du*

Pd-catalyzed asymmetric aminations of butadiene monoxide with isatin derivatives using P/alkene ligands gave high yields, ees and regioselectivity ratios.